LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016638.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.512	44	47	63	rVB	25761	62268	22.31%	1.349%
2	3.834	78	82	88	rBV	6631	14318	5.13%	0.310%
3	4.249	124	127	129	rBV	4460	6939	2.49%	0.150%
4	4.821	186	189	197	rVB	78274	152144	54.50%	3.296%
5	5.051	210	214	220	rBV	5565	13488	4.83%	0.292%
6	5.273	235	238	249	rVB	22106	47049	16.85%	1.019%
7	5.752	287	290	299	rVB2	4552	10973	3.93%	0.238%
8	6.656	384	388	391	rBV2	6475	12626	4.52%	0.273%
9	6.831	403	407	421	rVB	22934	46562	16.68%	1.009%
10	7.246	449	452	460	rVB2	6688	18971	6.80%	0.411%
11	7.643	490	495	499	rBV	58933	109313	39.16%	2.368%
12	7.707	499	502	506	rVB	5412	8455	3.03%	0.183%
13	7.864	516	519	523	rBV	7204	14138	5.06%	0.306%
14	7.938	523	527	533	rVB	70566	121311	43.46%	2.628%
15	8.177	549	553	559	rVB2	3643	8812	3.16%	0.191%
16	8.306	565	567	569	rVB	9334	9165	3.28%	0.199%
17	8.455	574	579	580	rVV2	1903	4857	1.74%	0.105%
18	8.493	580	582	586	rVB2	2564	4962	1.78%	0.107%
19	8.785	602	605	610	rVB	28566	52355	18.75%	1.134%
20	8.949	616	618	622	rVB	5819	9382	3.36%	0.203%
21	9.342	646	649	658	rVB2	1859	5138	1.84%	0.111%
22	9.824	684	687	691	rVB2	2155	4312	1.54%	0.093%
23	9.951	692	697	703	rBV6	962	4363	1.56%	0.095%
24	10.065	703	706	713	rBV2	4720	11805	4.23%	0.256%
25	10.191	713	716	720	rBV	147789	276506	99.05%	5.989%
26	10.407	729	733	736	rBV	114768	198130	70.97%	4.292%
27	10.457	736	737	739	rVV	7832	9970	3.57%	0.216%
28	10.508	739	741	745	rVB	5856	10068	3.61%	0.218%
29	10.774	759	762	764	rBV	3141	6372	2.28%	0.138%
30	11.205	794	796	802	rVB2	1868	3825	1.37%	0.083%
31	12.003	921	931	941	rBV2	48696	78827	28.24%	1.707%
32	12.078	941	948	962	rVB	5358	8663	3.10%	0.188%
33	12.296	987	997	1009	rVB	4822	7879	2.82%	0.171%
34	12.619	1050	1053	1059	rVB	2016	4042	1.45%	0.088%
35	12.899	1071	1075	1078	rBV2	83669	158302	56.71%	3.429%
36	13.178	1094	1097	1104	rBV2	18818	39923	14.30%	0.865%

LSC Area Percent Report

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Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.584	1127	1129	1132	rBV	3038	4986	1.79%	0.108%
38	13.990	1158	1161	1163	rBV	3430	5391	1.93%	0.117%
39	14.142	1169	1173	1180	rVB3	2836	7314	2.62%	0.158%
40	14.269	1180	1183	1186	rBV	143400	210426	75.38%	4.558%
41	14.345	1186	1189	1192	rVV3	4620	11083	3.97%	0.240%
42	14.434	1193	1196	1199	rVV	7350	10629	3.81%	0.230%
43	14.523	1199	1203	1206	rVV3	6864	15191	5.44%	0.329%
44	14.599	1206	1209	1212	rVB	4492	7029	2.52%	0.152%
45	14.751	1219	1221	1223	rBV	3443	4944	1.77%	0.107%
46	14.814	1223	1226	1229	rVB2	2054	4761	1.71%	0.103%
47	14.891	1229	1232	1235	rBV2	2806	6056	2.17%	0.131%
48	15.106	1243	1249	1251	rVB3	2347	5701	2.04%	0.123%
49	15.322	1263	1266	1268	rBV3	4705	8343	2.99%	0.181%
50	15.639	1287	1291	1295	rBV3	3428	10249	3.67%	0.222%
51	15.715	1295	1297	1299	rVV	10663	20140	7.21%	0.436%
52	15.766	1299	1301	1305	rVV2	13652	23639	8.47%	0.512%
53	15.855	1305	1308	1311	rVB3	2231	4581	1.64%	0.099%
54	16.007	1317	1320	1322	rVB	28512	34263	12.27%	0.742%
55	16.835	1386	1388	1394	rVB	4498	8310	2.98%	0.180%
56	17.018	1400	1403	1405	rBV	107083	170502	61.08%	3.693%
57	17.066	1405	1407	1410	rVV	27459	39527	14.16%	0.856%
58	17.152	1411	1414	1417	rVB	5019	9117	3.27%	0.197%
59	17.225	1417	1420	1425	rBV	5120	12897	4.62%	0.279%
60	17.431	1434	1437	1443	rVB2	2641	4604	1.65%	0.100%
61	17.784	1463	1466	1474	rVB	7125	14254	5.11%	0.309%
62	17.955	1474	1480	1483	rBV2	8812	21483	7.70%	0.465%
63	18.909	1661	1665	1674	rVB	8785	11931	4.27%	0.258%
64	19.063	1688	1696	1700	rBV	105913	152039	54.46%	3.293%
65	19.098	1700	1703	1713	rVB	64799	79190	28.37%	1.715%
66	19.242	1728	1732	1745	rBV2	6427	9766	3.50%	0.212%
67	19.460	1767	1776	1788	rBV	61129	85303	30.56%	1.848%
68	19.679	1814	1820	1836	rVB	87773	114286	40.94%	2.476%
69	19.783	1837	1841	1847	rBV	3553	4818	1.73%	0.104%
70	20.006	1884	1886	1888	rBV	8961	10662	3.82%	0.231%
71	20.378	1918	1921	1924	rBV	88499	102947	36.88%	2.230%
72	20.537	1934	1936	1940	rVB	7650	11226	4.02%	0.243%
73	20.718	1951	1953	1957	rBV4	2914	6529	2.34%	0.141%
74	20.803	1960	1961	1963	rBV	2828	3760	1.35%	0.081%
75	20.866	1965	1967	1970	rVB2	11571	18878	6.76%	0.409%
76	20.920	1970	1972	1973	rBV	3554	4694	1.68%	0.102%

LSC Area Percent Report

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Operator : CG/JU
Sample : M4020-16
Misc :
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Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	20.973	1974	1977	1984	rVB3	30508	60314	21.61%	1.306%
78	21.174	1993	1996	1998	rBV2	27432	52822	18.92%	1.144%
79	21.228	1998	2001	2004	rVV2	153558	273301	97.90%	5.920%
80	21.270	2004	2005	2011	rVB	36998	35558	12.74%	0.770%
81	21.684	2042	2044	2047	rVB	6357	9610	3.44%	0.208%
82	21.748	2047	2050	2052	rBV	6083	11071	3.97%	0.240%
83	21.875	2057	2062	2065	rBV2	186688	279159	100.00%	6.047%
84	22.003	2071	2074	2077	rBV	119198	159497	57.13%	3.455%
85	22.067	2077	2080	2081	rVV	21695	33311	11.93%	0.722%
86	22.109	2081	2084	2088	rVB2	81680	113541	40.67%	2.459%
87	22.311	2100	2103	2109	rVV2	24996	63413	22.72%	1.374%
88	22.396	2109	2111	2113	rVB	12878	13140	4.71%	0.285%
89	22.807	2220	2229	2235	rBV	25528	50231	17.99%	1.088%
90	22.896	2249	2255	2270	rVB	12453	22973	8.23%	0.498%
91	22.978	2273	2279	2298	rVB3	7713	14762	5.29%	0.320%
92	23.286	2360	2369	2384	rVB2	16119	29861	10.70%	0.647%
93	23.382	2388	2397	2414	rVV2	19036	38926	13.94%	0.843%
94	23.481	2415	2426	2434	rVV	111764	216223	77.46%	4.684%
95	23.529	2434	2440	2465	rVB	79065	154138	55.22%	3.339%
96	24.084	2595	2602	2616	rVB	8087	15234	5.46%	0.330%
97	24.176	2619	2629	2652	rBV	18076	49480	17.72%	1.072%
98	25.473	2997	3008	3013	rBV3	1840	4237	1.52%	0.092%
99	25.761	3077	3092	3118	rVB3	12341	38245	13.70%	0.828%
100	26.459	3280	3296	3326	rBV	9498	29966	10.73%	0.649%

Sum of corrected areas: 4616675

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
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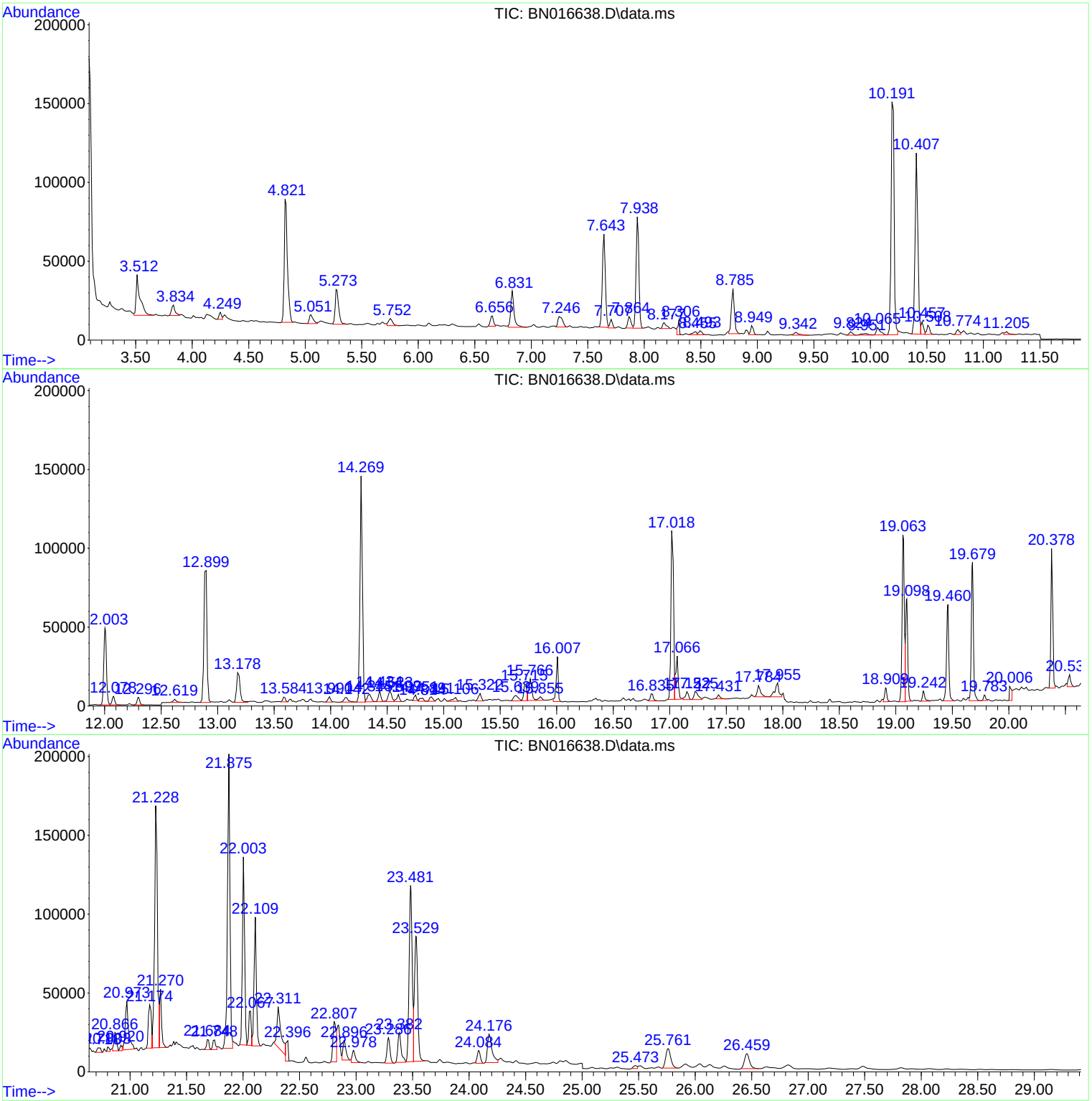
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

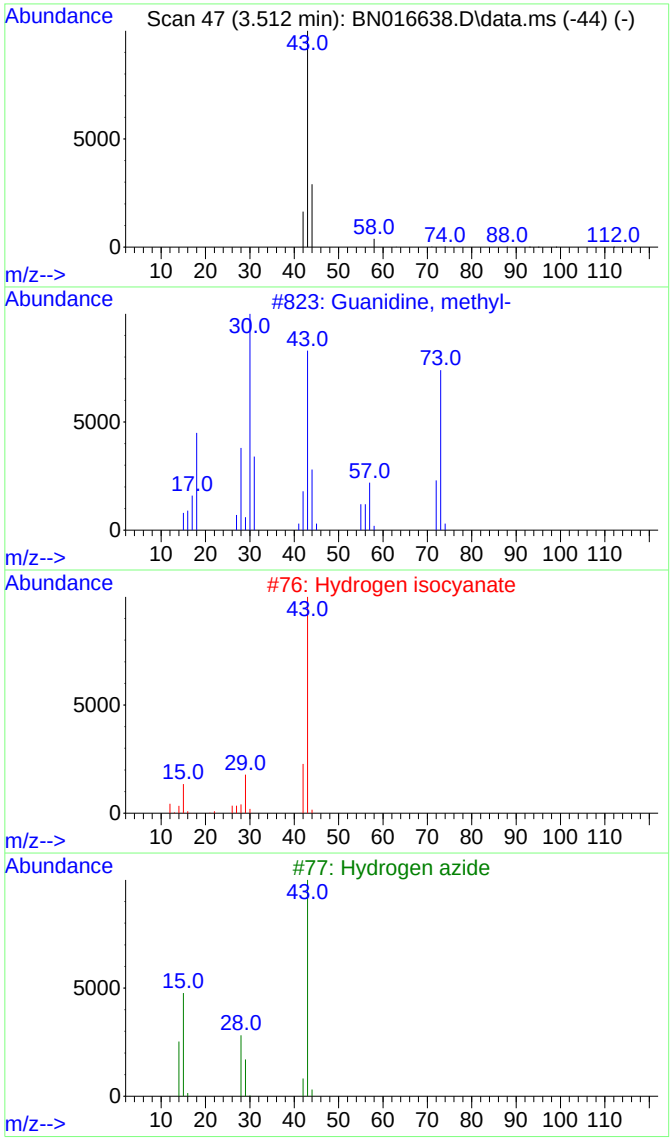
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

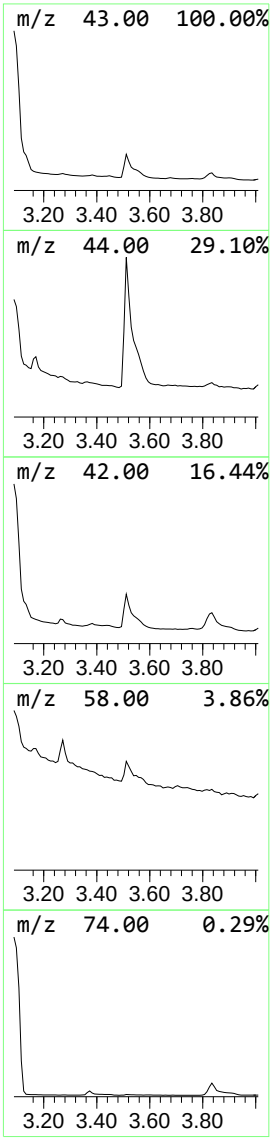
****

Peak Number 1 Guanidine, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.512	0.23 ng	62268	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
2	Hydrogen isocyanate	43	CHNO	000075-13-8	3
3	Hydrogen azide	43	HN3	007782-79-8	3
4	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	3
5	Isobutane	58	C4H10	000075-28-5	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

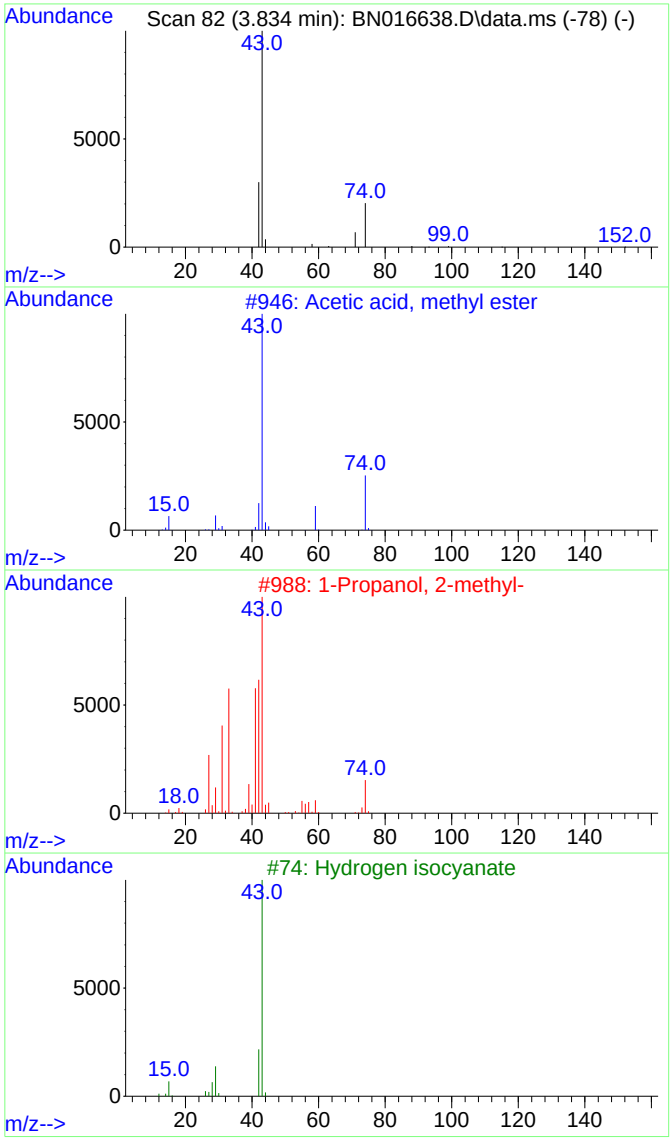
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

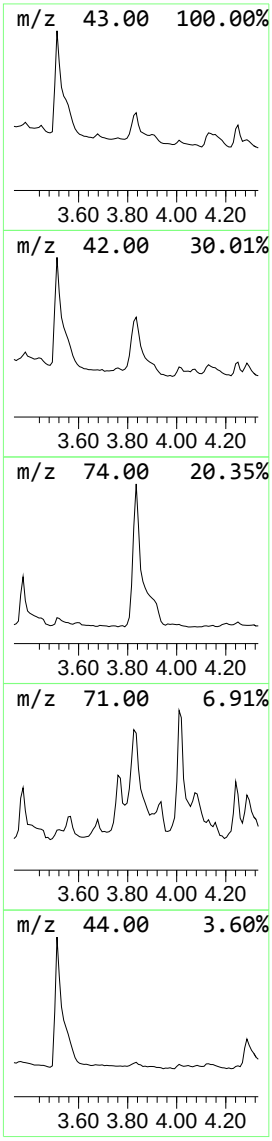
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, methyl ester Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.834	0.05 ng	14318	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	5
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Isobutane	58	C4H10	000075-28-5	4
5	Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
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Sample : M4020-16
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BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

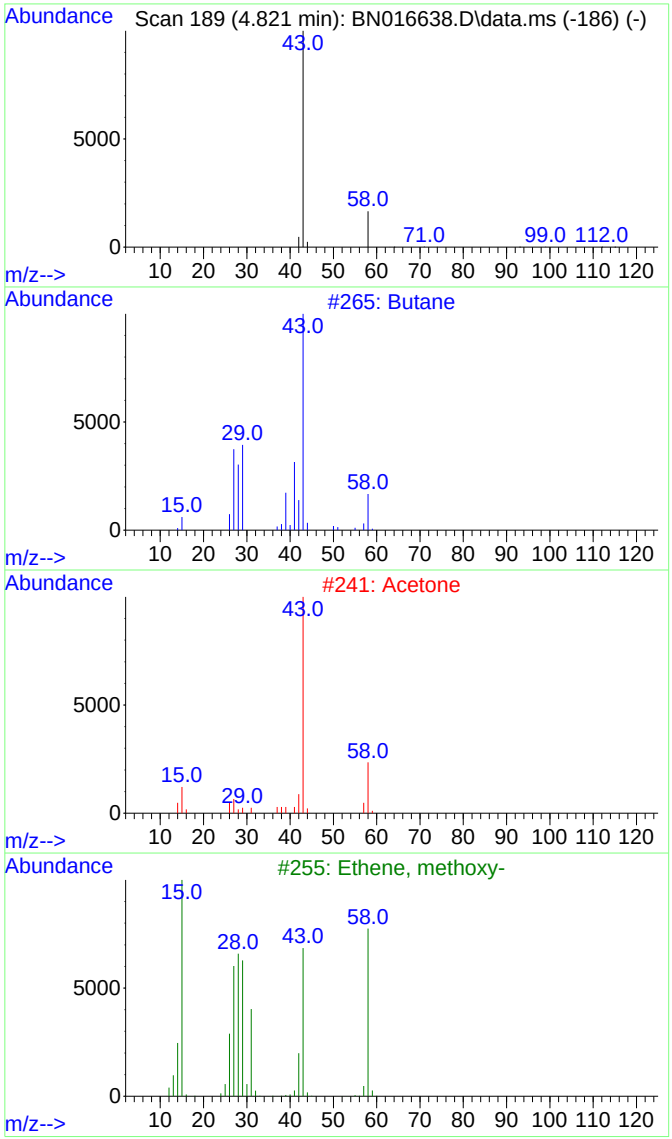
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

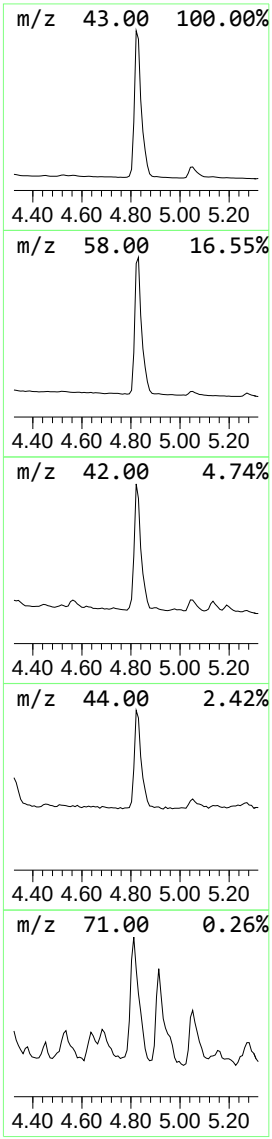
****

Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.56 ng	152144	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	Ethene, methoxy-	58	C3H6O	000107-25-5	3
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

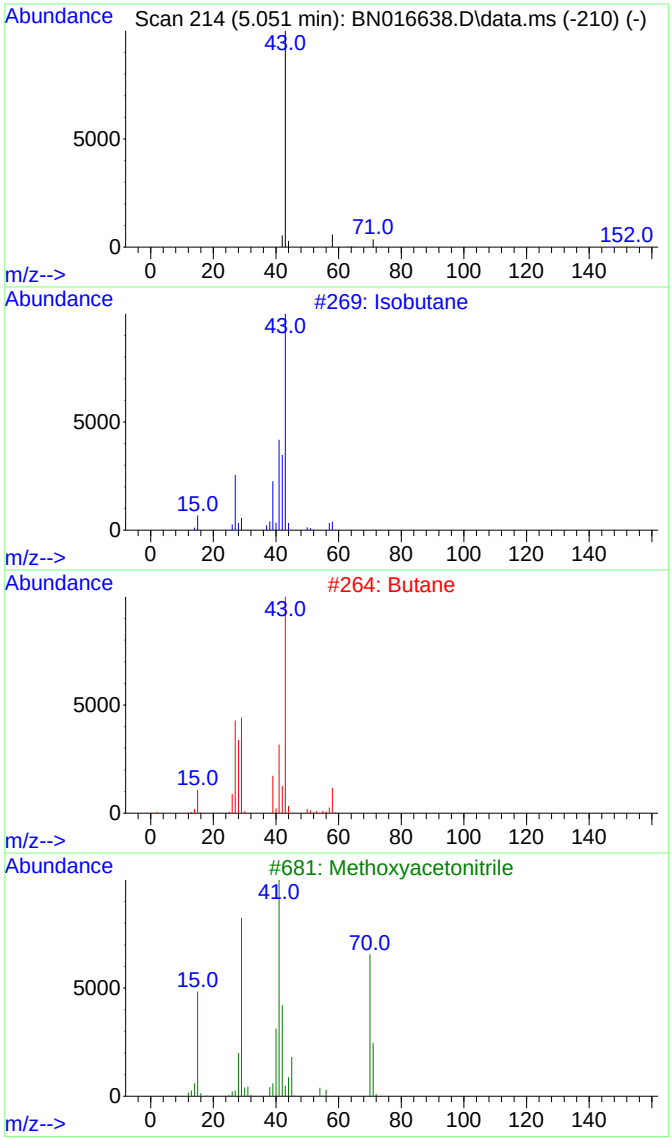
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

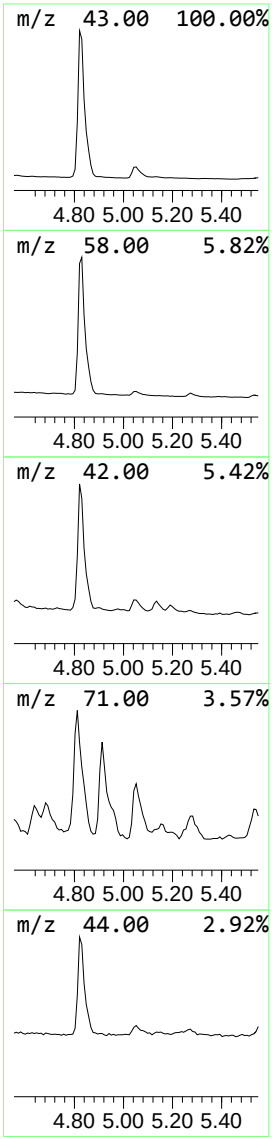
****

Peak Number 4 Isobutane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	0.05 ng	13488	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	4
2	Butane	58	C4H10	000106-97-8	3
3	Methoxyacetonitrile	71	C3H5NO	001738-36-9	2
4	Hydrogen isocyanate	43	CHNO	000075-13-8	2
5	Hydrogen azide	43	HN3	007782-79-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

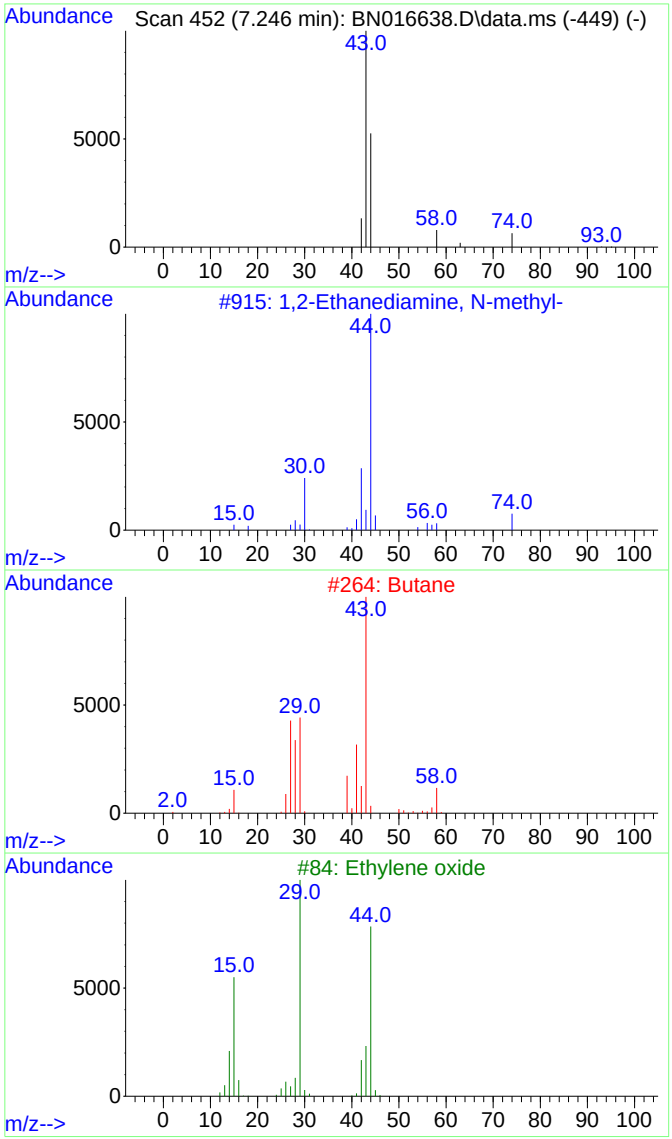
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

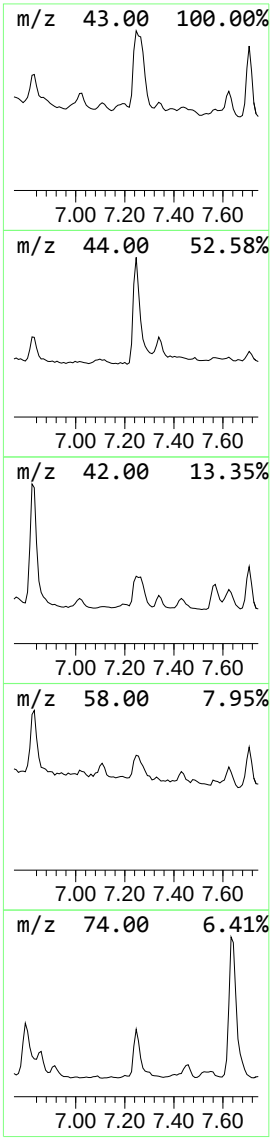
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,2-Ethanediamine, N-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.246	0.07 ng	18971	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediamine, N-methyl-	74	C3H10N2	000109-81-9	5
2	Butane	58	C4H10	000106-97-8	4
3	Ethylene oxide	44	C2H4O	000075-21-8	4
4	Acetaldehyde	44	C2H4O	000075-07-0	4
5	Propane	44	C3H8	000074-98-6	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

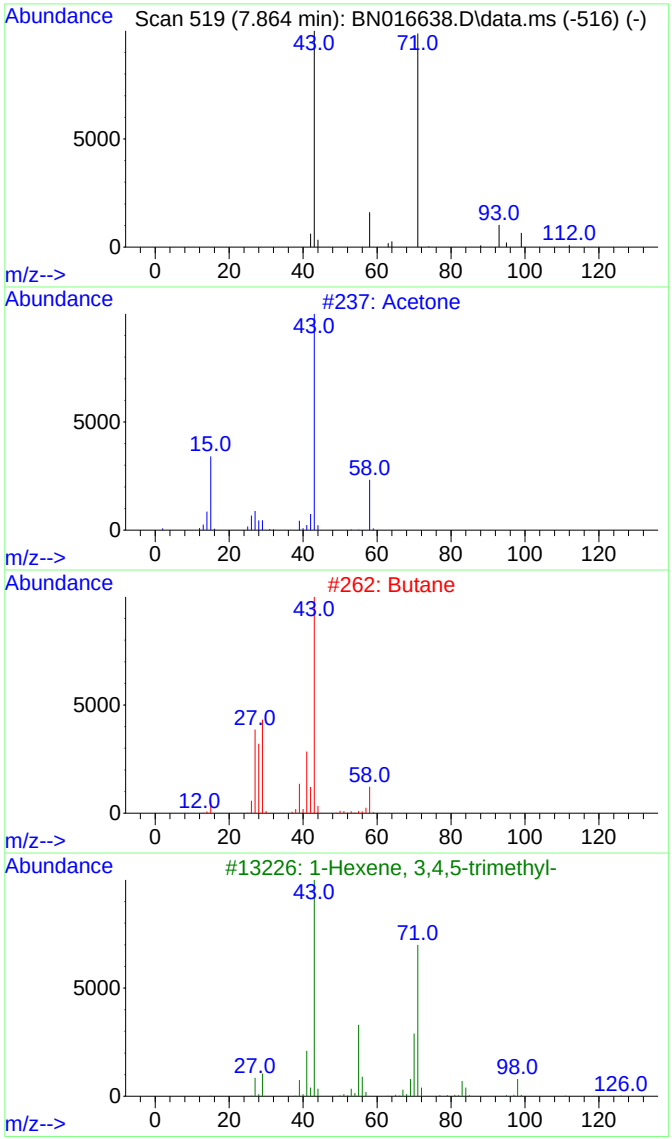
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

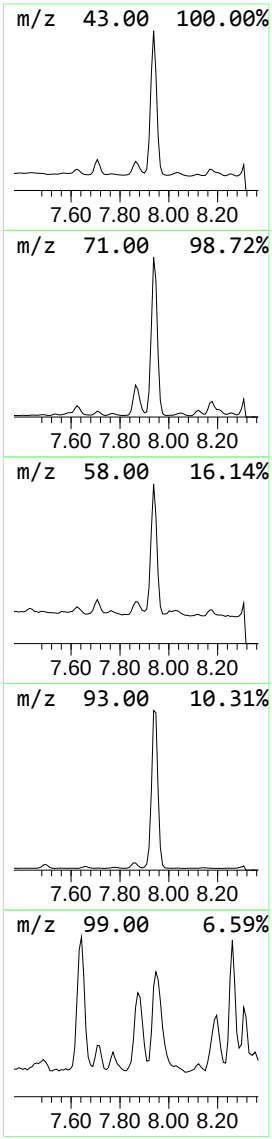
****

Peak Number 6 Acetone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.05 ng	14138	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone	58	C3H6O	000067-64-1	7
2	Butane	58	C4H10	000106-97-8	4
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	4





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Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

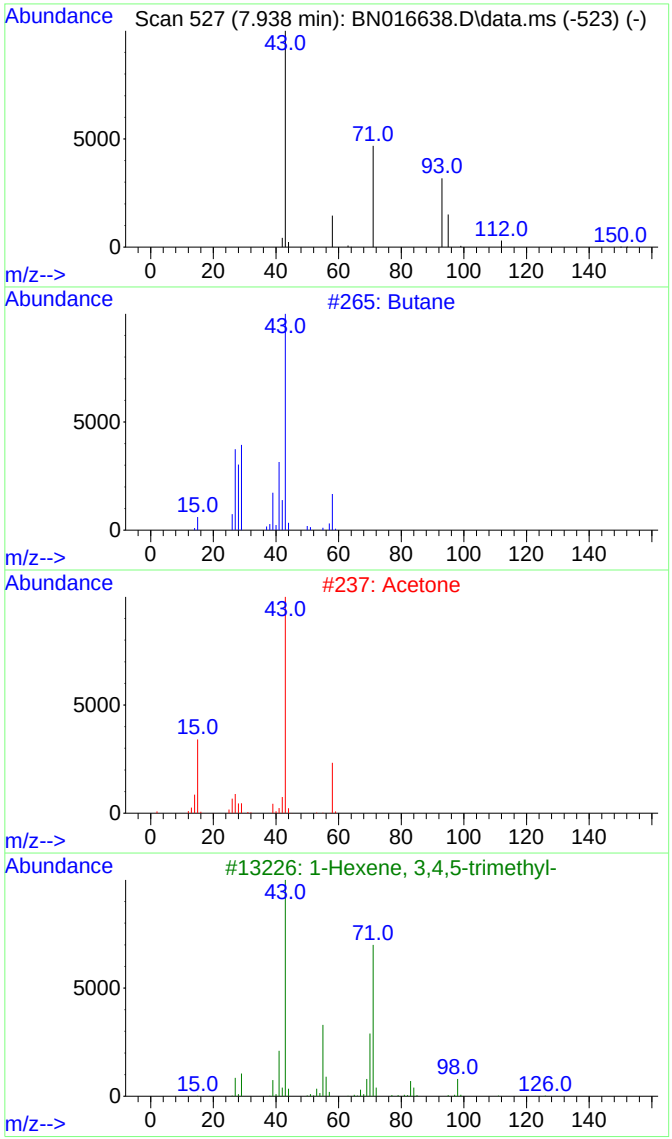
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

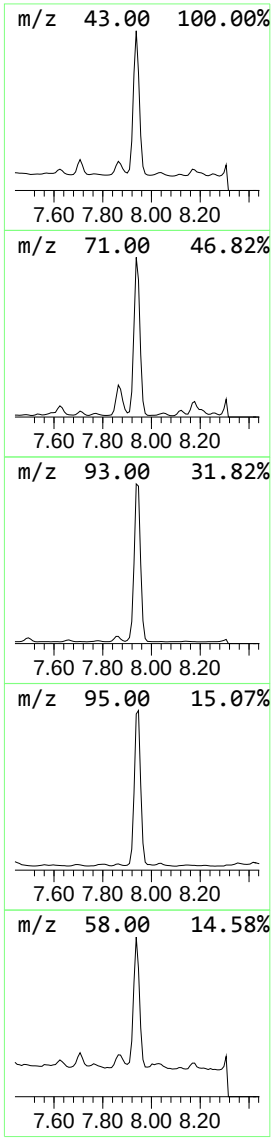
****

Peak Number 7 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.938	0.44 ng	121311	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	3
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3





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ClientSampleId :
S-821-N-SO-1-1.5-093021

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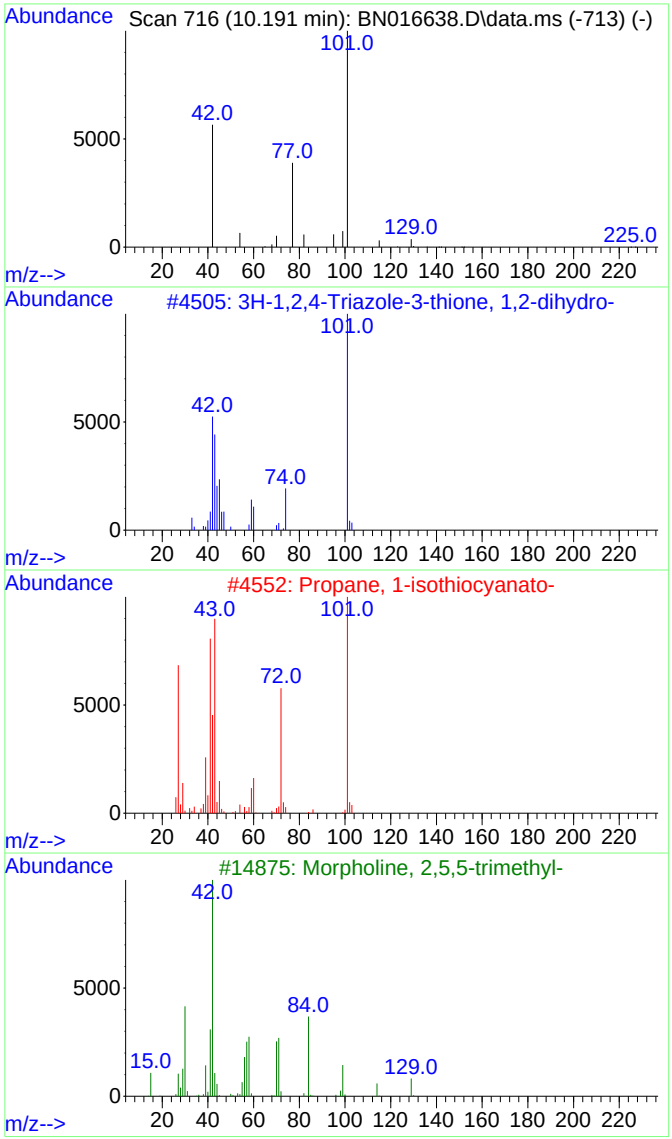
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

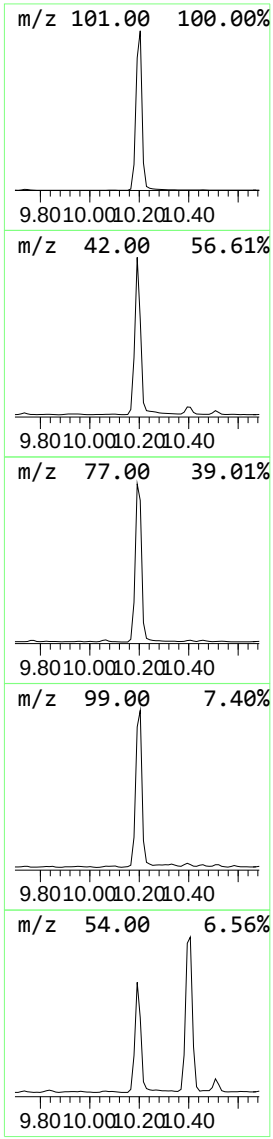
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 3H-1,2,4-Triazole-3-thione,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.56 ng	276506	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3	Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5
4	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
5	4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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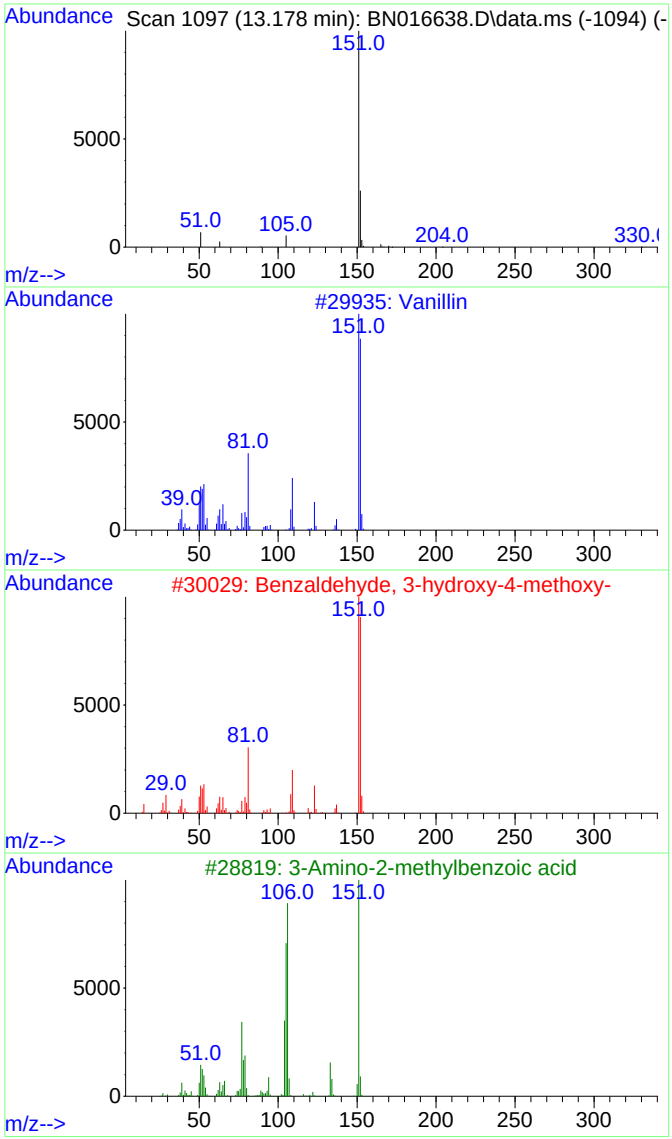
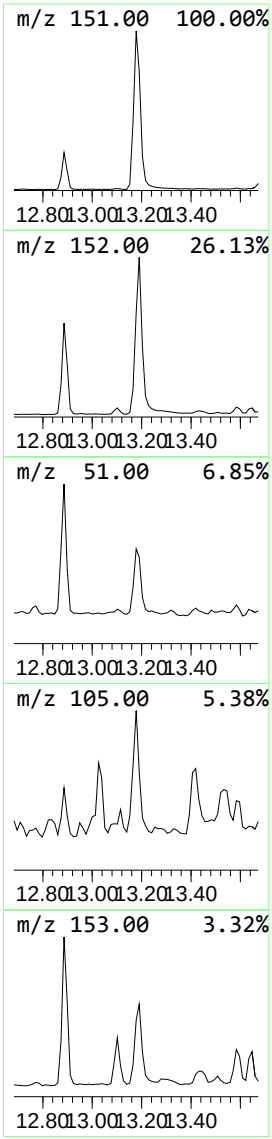
****
Peak Number 9 Vanillin Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.08 ng	39923	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	9
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	5
3	3-Amino-2-methylbenzoic acid	151	C8H9NO2	052130-17-3	4
4	Furane-2-carboxaldehyde, iminose...	152	C6H8N4O	004353-50-8	4
5	4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	4





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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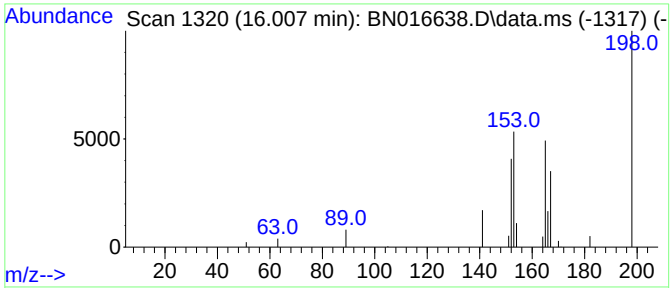
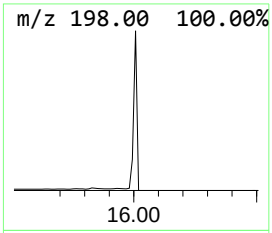
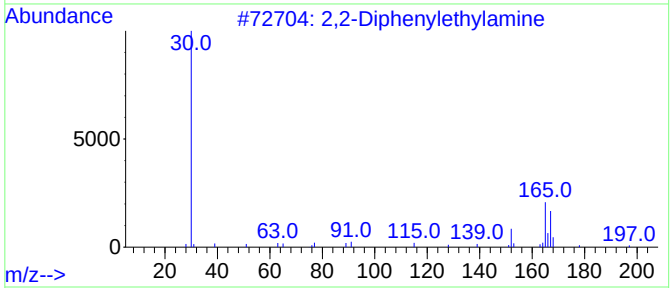
Peak Number 10 2,2-Diphenylethylamine Concentration Rank 12

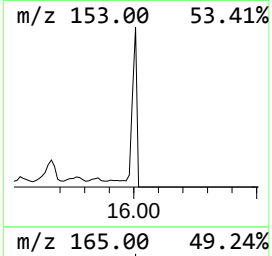
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.08 ng	34263	Phenanthrene-d10	17.018

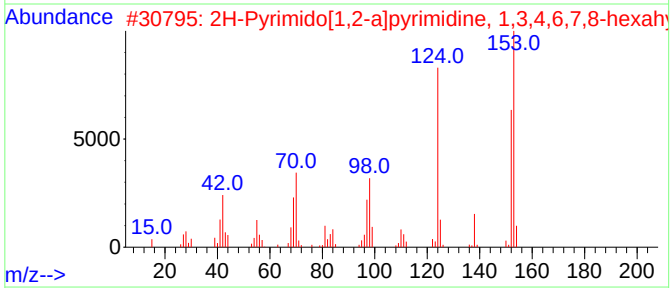
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Diphenylethylamine	197	C14H15N	003963-62-0	12
2	2H-Pyrimido[1,2-a]pyrimidine, 1,...	153	C8H15N3	084030-20-6	9
3	2(1H)-Pyridinethione, 1-ethyl-6-...	153	C8H11NS	019006-73-6	9
4	2,4-Dimethyl-6-(methylthio)pyridine	153	C8H11NS	1000305-54-7	9
5	Benzenethiol, p-(dimethylamino)-	153	C8H11NS	004946-22-9	9

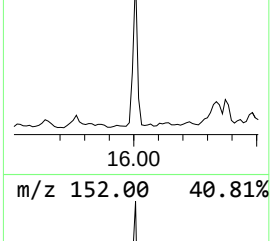


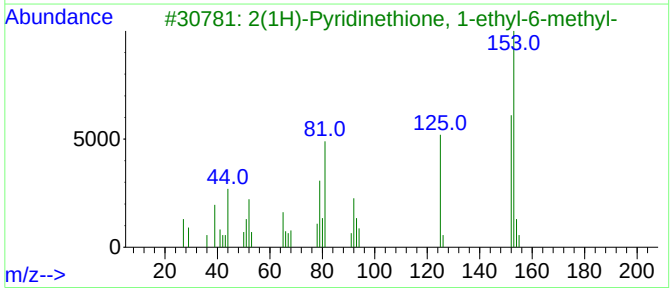


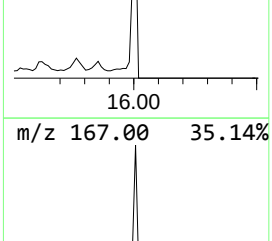












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Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

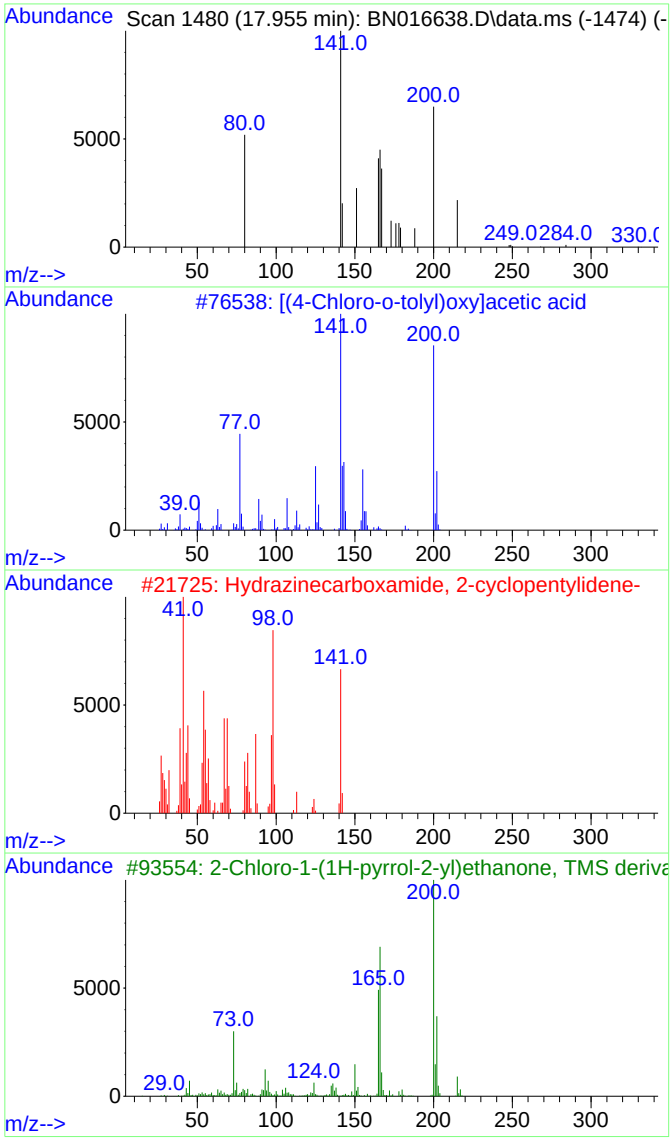
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

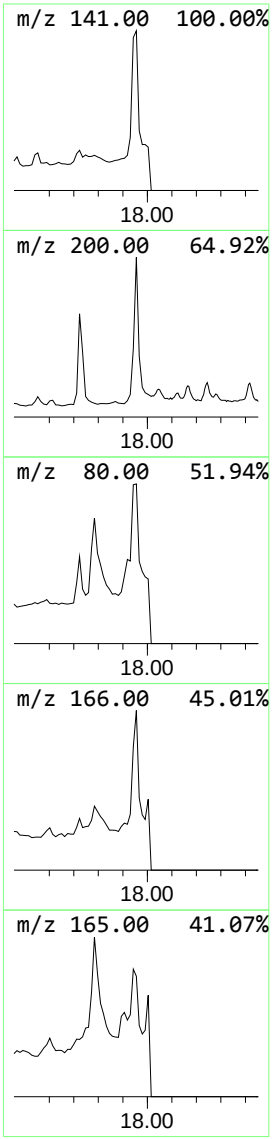
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 [(4-Chloro-o-tolyl)oxy]acet... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.955	0.05 ng	21483	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[(4-Chloro-o-tolyl)oxy]acetic acid	200	C9H9ClO3	000094-74-6	16
2	Hydrazinecarboxamide, 2-cyclopen...	141	C6H11N3O	005459-00-7	9
3	2-Chloro-1-(1H-pyrrol-2-yl)ethan...	215	C9H14ClNOSi	1000485-05-7	9
4	2-Cyclopentene-1,1-dicarboxylic ...	260	C15H16O4	1000460-72-1	9
5	Isothiocyanic acid, hexamethylen...	200	C8H12N2S2	005586-70-9	7





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Misc :
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Instrument : BNA_N
ClientSampleId : S-821-N-SO-1-1.5-093021

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

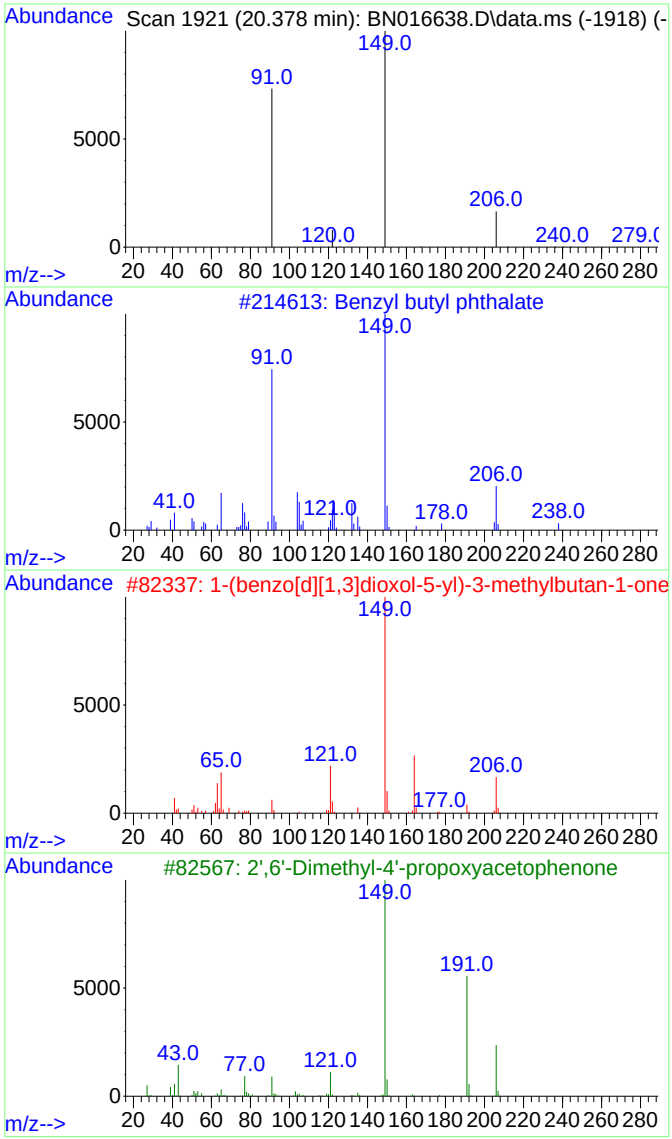
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

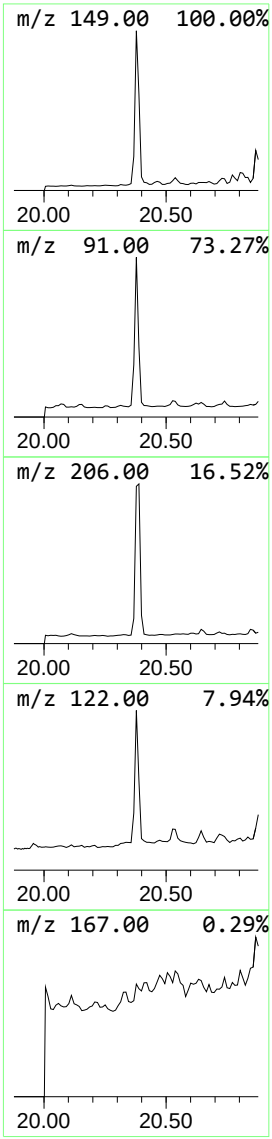
****

Peak Number 12 Benzyl butyl phthalate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.15 ng	102947	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl butyl phthalate	312	C19H20O4	000085-68-7	43
2	1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3	2',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4	2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	5
5	2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5





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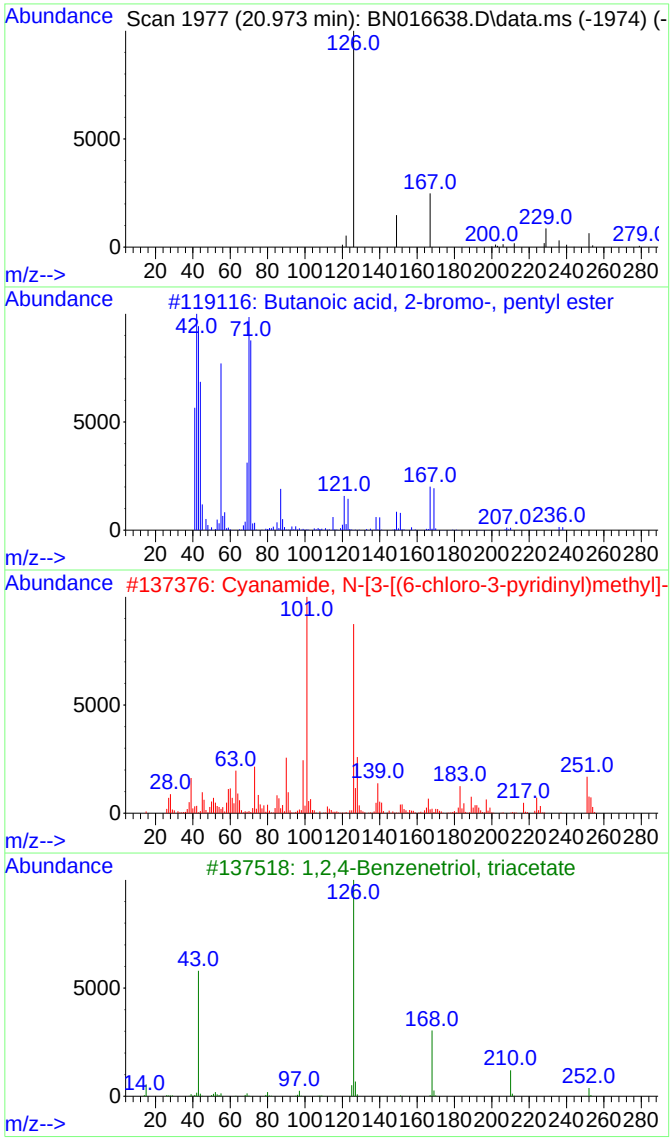
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

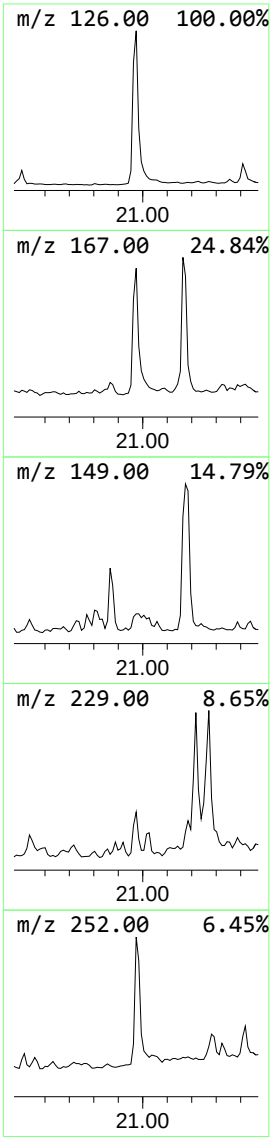
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Butanoic acid, 2-bromo-, pe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.09 ng	60314	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-bromo-, pentyl ...	236	C9H17BrO2	1000131-81-8	5
2	Cyanamide, N-[3-[(6-chloro-3-pyr...	252	C10H9ClN4S	111988-49-9	4
3	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
4	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
5	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4





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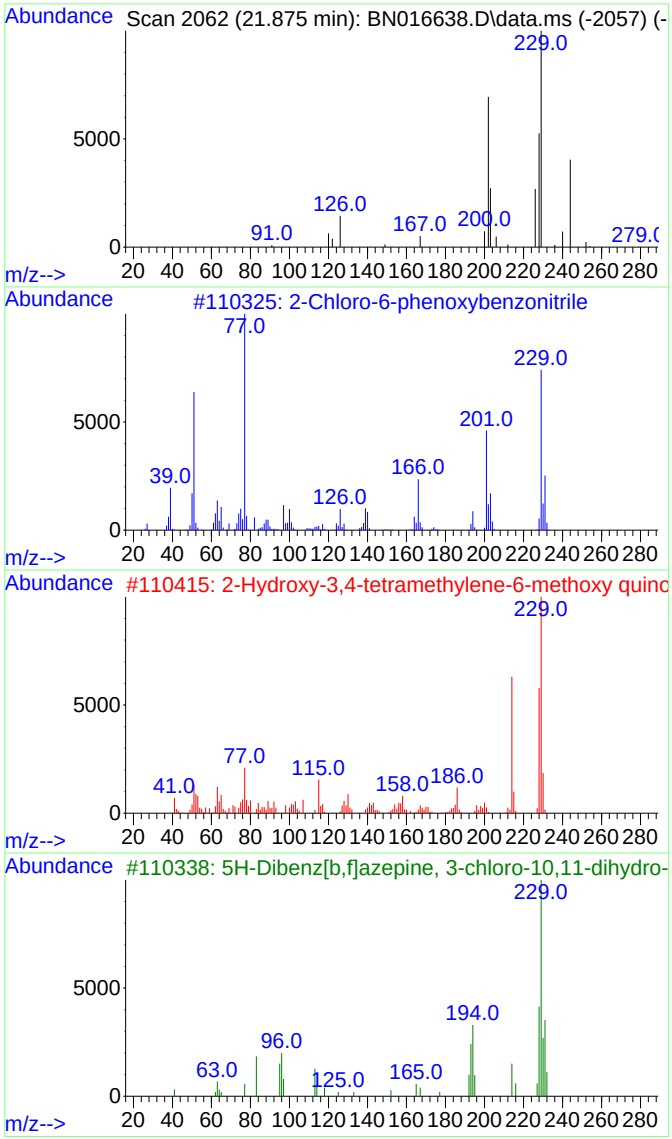
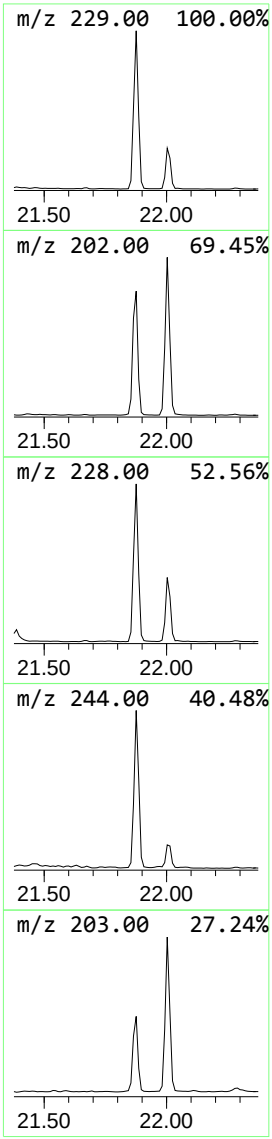
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2-Chloro-6-phenoxybenzonitrile Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.875	0.41 ng	279159	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-6-phenoxybenzonitrile	229	C13H8ClNO	1000340-54-1	25
2	2-Hydroxy-3,4-tetramethylene-6-m...	229	C14H15NO2	004562-57-6	17
3	5H-Dibenz[b,f]azepine, 3-chloro-...	229	C14H12ClN	032943-25-2	9
4	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	9
5	2-Propenoic acid, 2-cyano-3-[4-(...	244	C14H16N2O2	1000115-72-8	9





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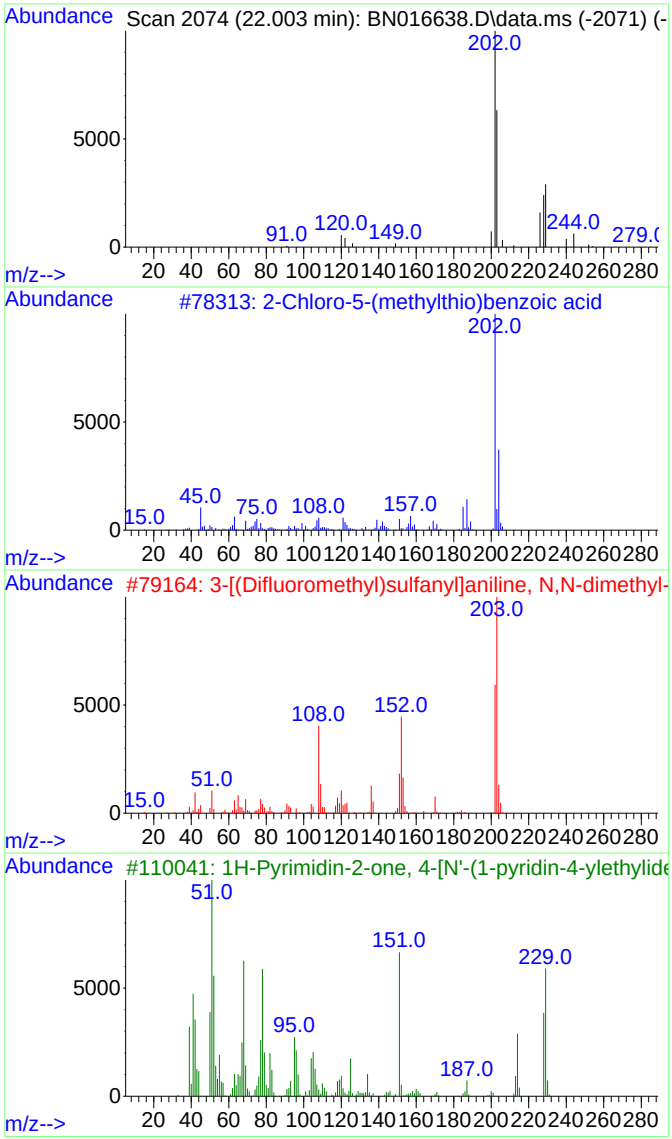
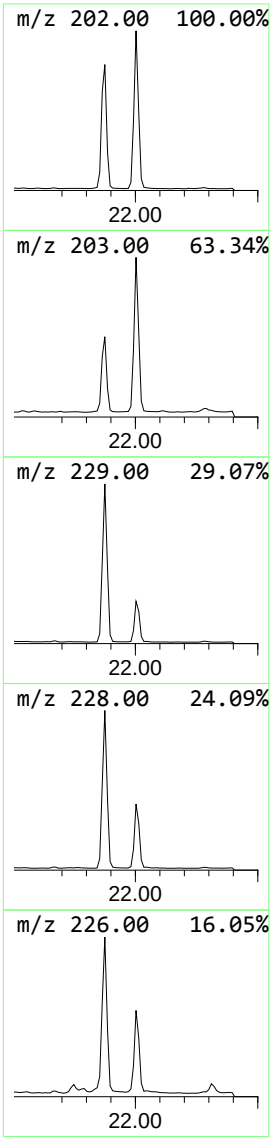
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 2-Chloro-5-(methylthio)benz... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.003	0.23 ng	159497	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-5-(methylthio)benzoic acid	202	C8H7ClO2S	051546-12-4	7
2	3-[(Difluoromethyl)sulfanyl]anil...	203	C9H11F2NS	1000505-37-1	7
3	1H-Pyrimidin-2-one, 4-[N'-(1-pyr...	229	C11H11N5O	1000304-67-8	7
4	2,3-Dichlorophenyl isothiocyanate	203	C7H3Cl2NS	006590-97-2	5
5	9-Cyanophenanthrene	203	C15H9N	002510-55-6	5





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Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

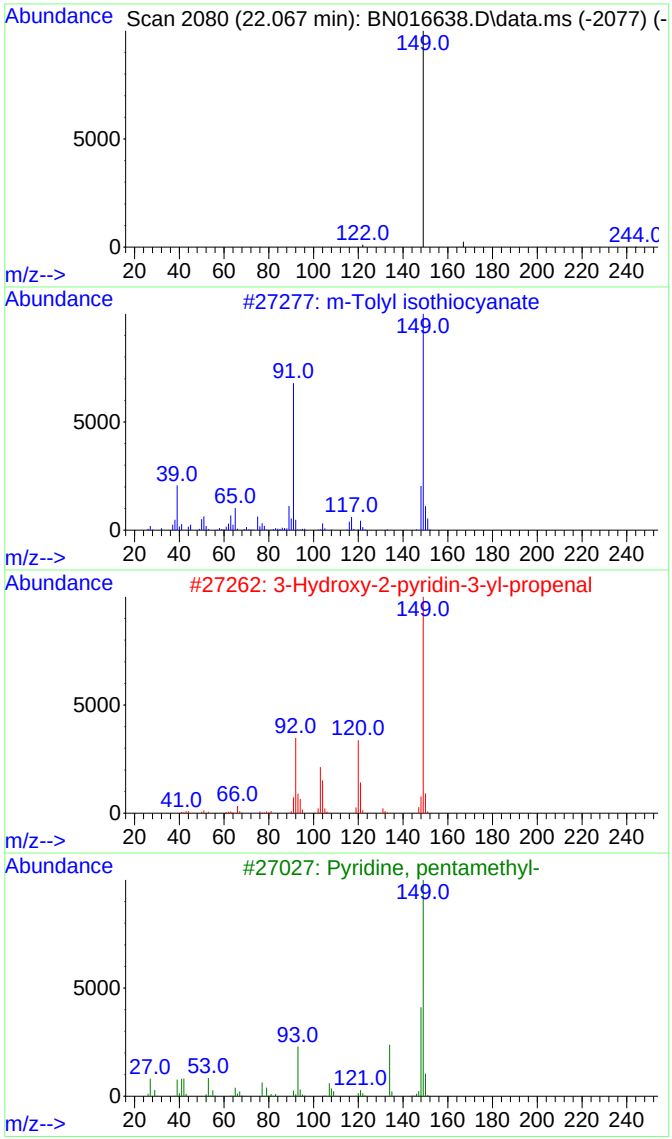
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

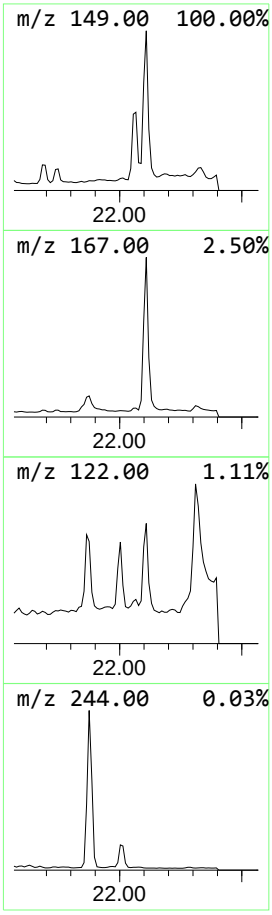
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 m-Tolyl isothiocyanate Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.067	0.05 ng	33311	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
2	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





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Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

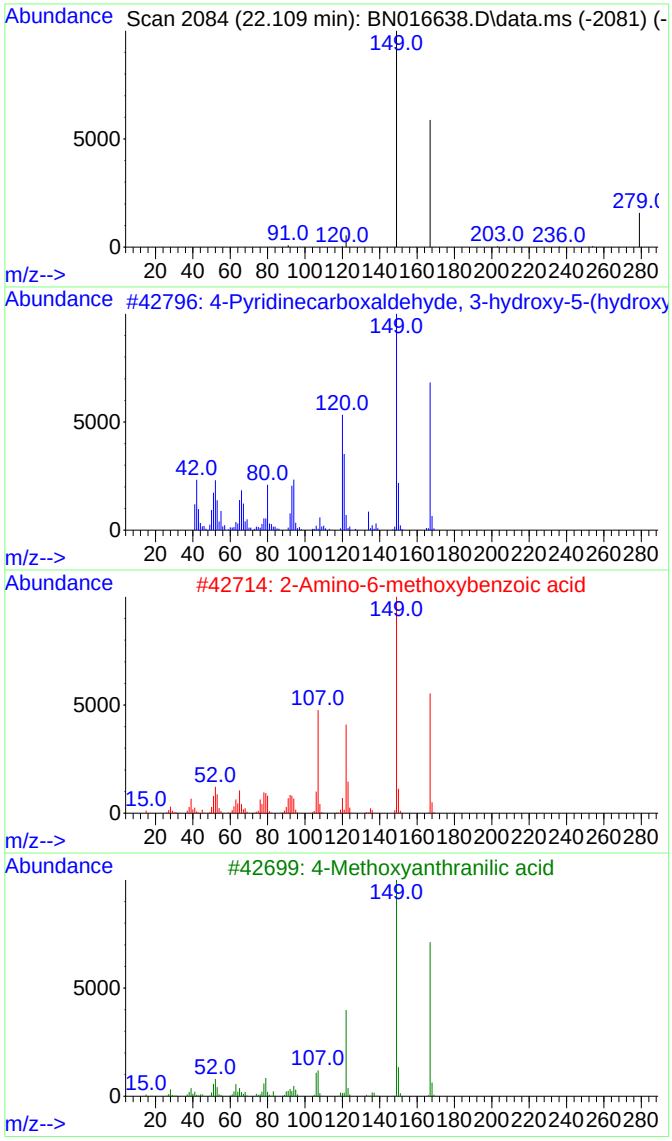
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

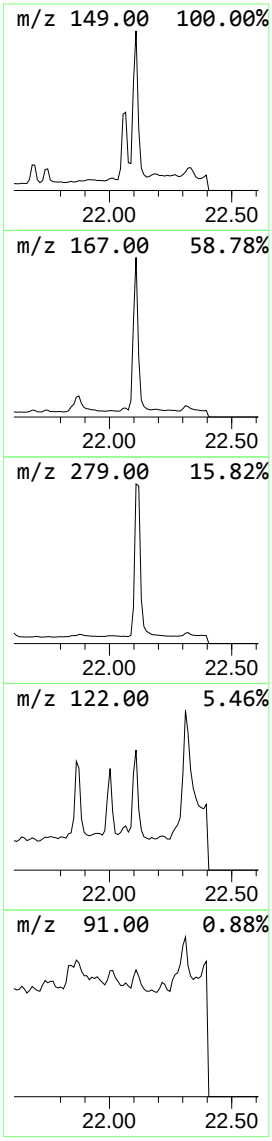
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 4-Pyridinecarboxaldehyde, 3... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.109	0.17 ng	113541	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	9
2	2-Amino-6-methoxybenzoic acid	167	C8H9NO3	1000496-75-6	5
3	4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	5
4	6H-Thieno[2,3-b]pyrrole-5-carbox...	167	C7H5NO2S	051856-25-8	5
5	Nicotinic acid, 1,2-dihydro-4,6-...	167	C8H9NO3	024667-09-2	5





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Data File : BN016638.D
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Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

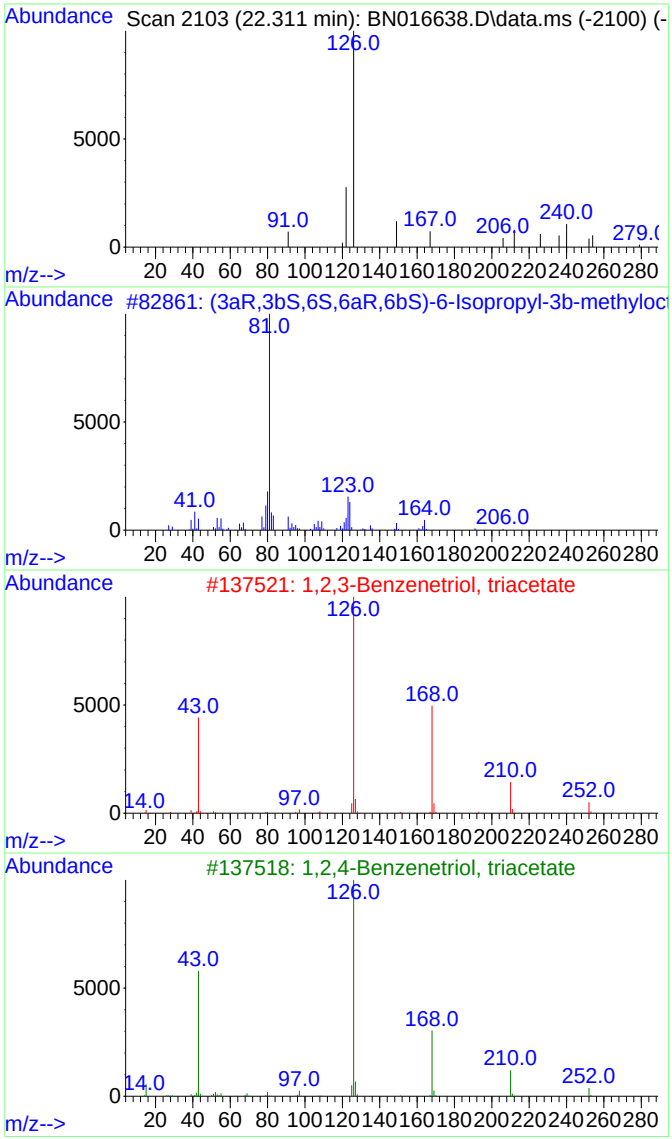
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

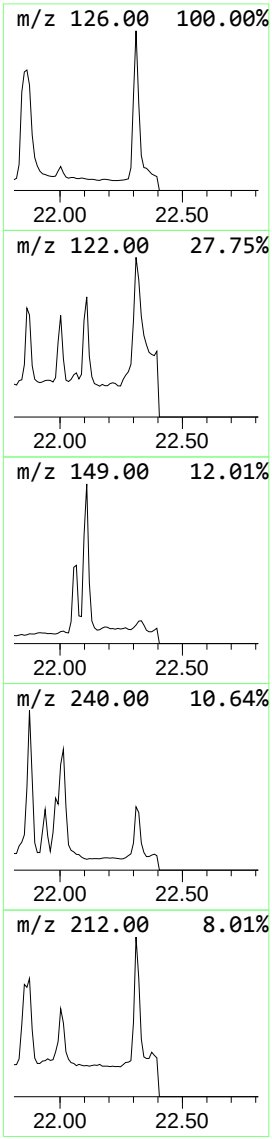
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 (3aR,3bS,6S,6aR,6bS)-6-Isop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.311	0.09 ng	63413	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3aR,3bS,6S,6aR,6bS)-6-Isopropyl...	206	C14H22O	013844-03-6	4
2	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
3	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
4	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
5	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4





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Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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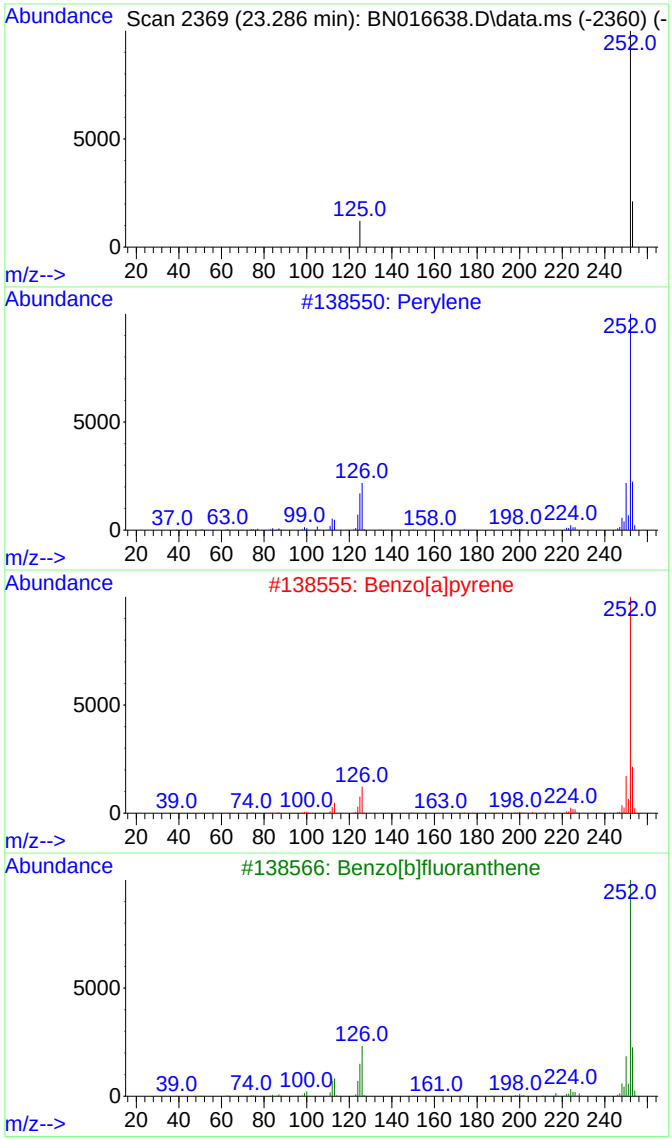
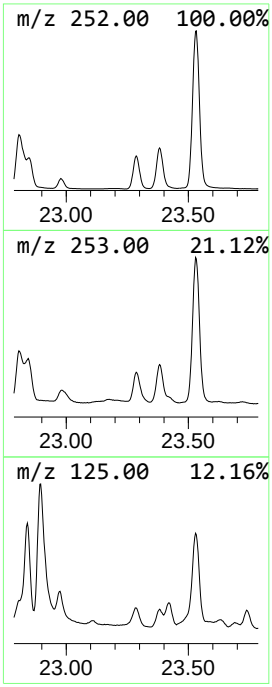
Peak Number 19 Perylene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.286	0.06 ng	29861	Perylene-d12	23.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	9
2	Benzo[a]pyrene	252	C20H12	000050-32-8	9
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
5	Gama-carbolin-1-one, 5,7-difluor...	252	C12H10F2N2O2	062223-53-4	9





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Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

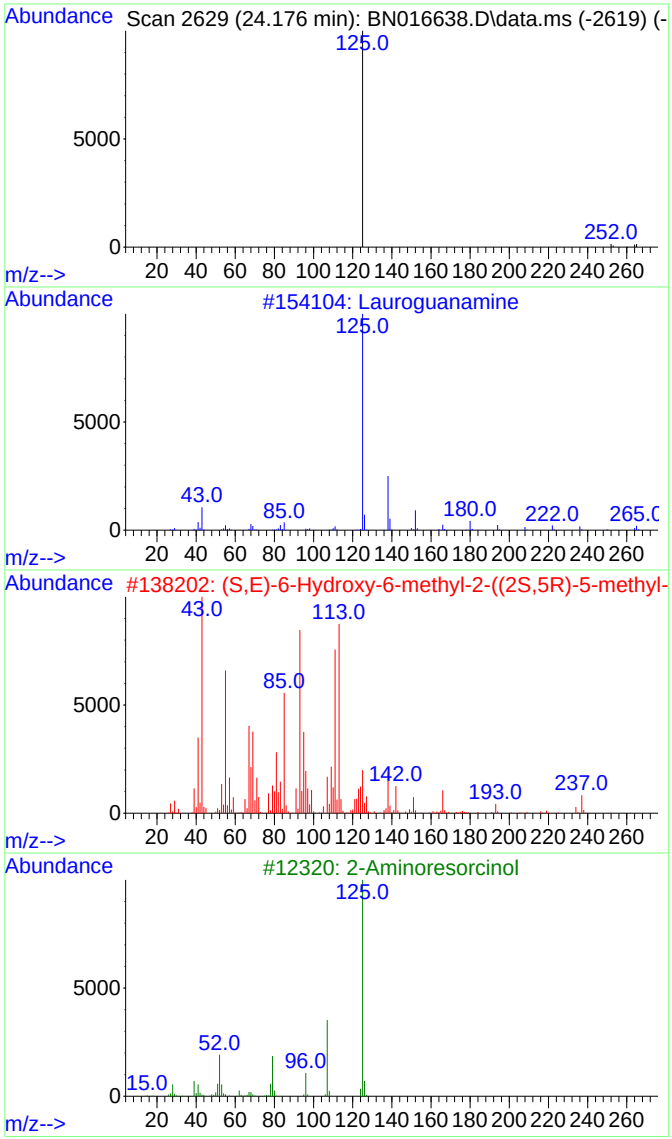
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

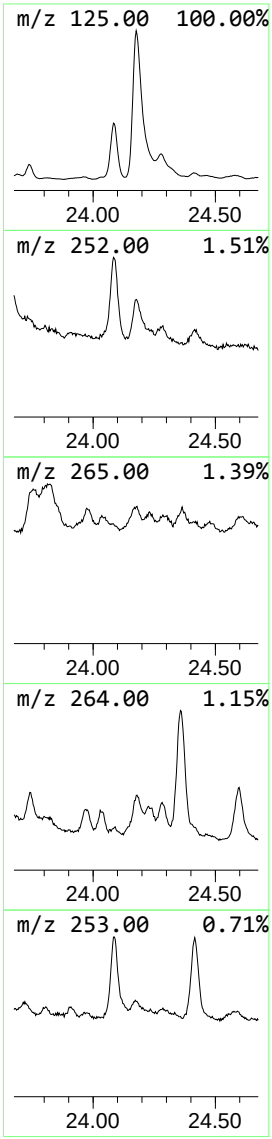
****

Peak Number 20 Lauroguanamine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.176	0.09 ng	49480	Perylene-d12	23.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lauroguanamine	265	C14H27N5	002533-34-8	5
2	(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3
3	2-Aminoresorcinol	125	C6H7NO2	003163-15-3	2
4	2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	2
5	2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016638.D
Acq On : 01 Oct 2021 16:32
Operator : CG/JU
Sample : M4020-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-1-1.5-093021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Guanidine, methyl-	3.512	0.2	ng	62268	1	7.643	109313	0.4
Acetic acid, me...	3.834	0.1	ng	14318	1	7.643	109313	0.4
Butane	4.821	0.6	ng	152144	1	7.643	109313	0.4
Isobutane	5.051	0.0	ng	13488	1	7.643	109313	0.4
1,2-Ethanediami...	7.246	0.1	ng	18971	1	7.643	109313	0.4
Acetone	7.864	0.1	ng	14138	1	7.643	109313	0.4
Butane	7.938	0.4	ng	121311	1	7.643	109313	0.4
3H-1,2,4-Triazo...	10.191	0.6	ng	276506	2	10.407	198130	0.4
Vanillin	13.178	0.1	ng	39923	3	14.269	210426	0.4
2,2-Diphenyleth...	16.007	0.1	ng	34263	4	17.018	170502	0.4
[(4-Chloro-o-to...	17.955	0.1	ng	21483	4	17.018	170502	0.4
Benzyl butyl ph...	20.378	0.2	ng	102947	5	21.227	273301	0.4
Butanoic acid, ...	20.973	0.1	ng	60314	5	21.227	273301	0.4
2-Chloro-6-phen...	21.875	0.4	ng	279159	5	21.227	273301	0.4
2-Chloro-5-(met...	22.003	0.2	ng	159497	5	21.227	273301	0.4
m-Tolyl isothio...	22.067	0.0	ng	33311	5	21.227	273301	0.4
4-Pyridinecarbo...	22.109	0.2	ng	113541	5	21.227	273301	0.4
(3aR,3bS,6S,6aR...	22.311	0.1	ng	63413	5	21.227	273301	0.4
Perylene	23.286	0.1	ng	29861	6	23.481	216223	0.4
Lauroguanamine	24.176	0.1	ng	49480	6	23.481	216223	0.4